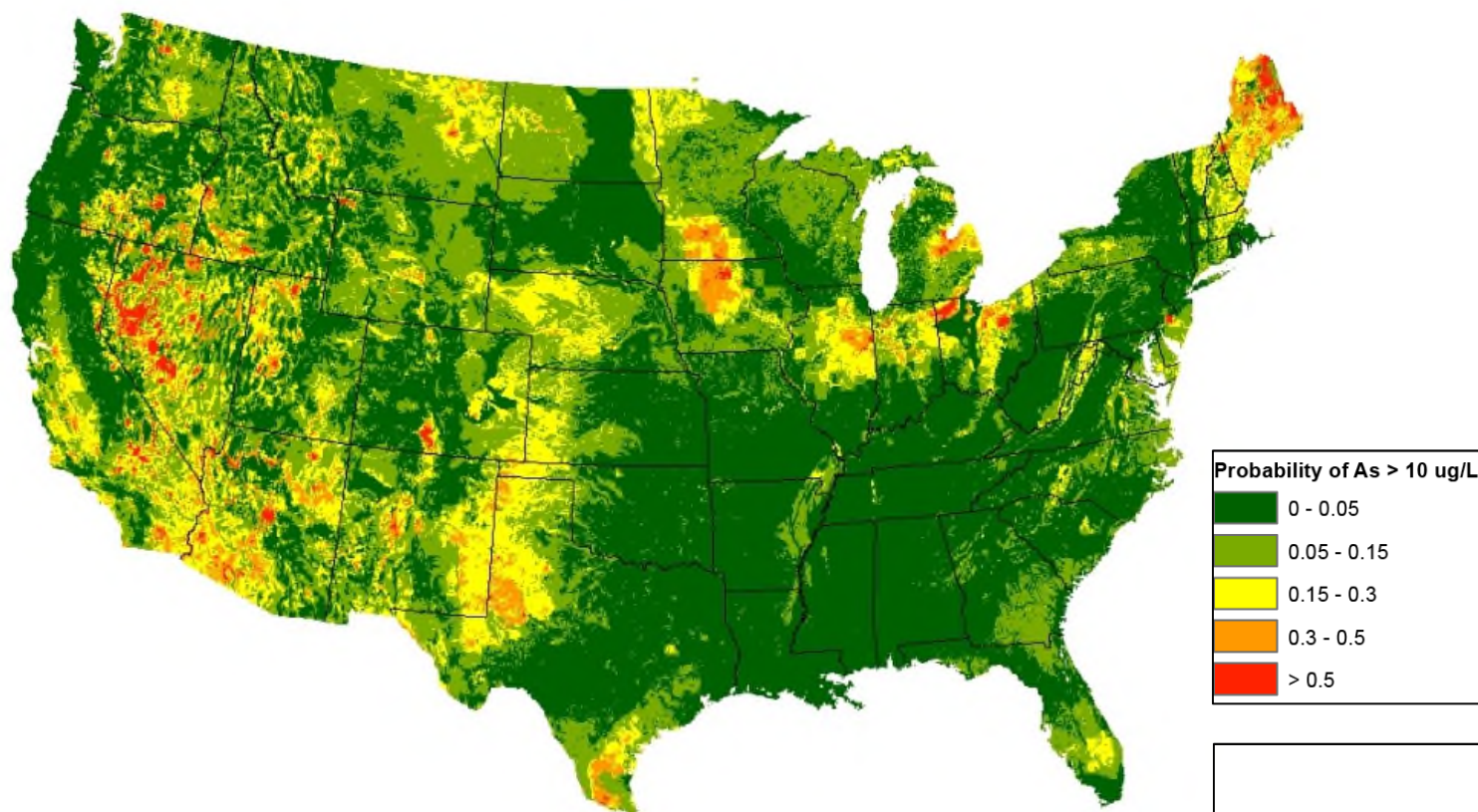# A comparison of statistical modeling techniques to predict arsenic in domestic wells in the CONUS

Melissa Lombard, Bernard T. Nolan, Mathew Gribble, Maria Argos, Joseph Ayotte

Estimating the High-Arsenic Domestic-Well Population in the Conterminous United States

Joseph D. Ayotte,[*,†] Laura Medalie,[‡] Sharon L. Qi,[§] Lorraine C. Backer,[∥] and Bernard T. Nolan[⊥]

Probability of As > 10 ug/L
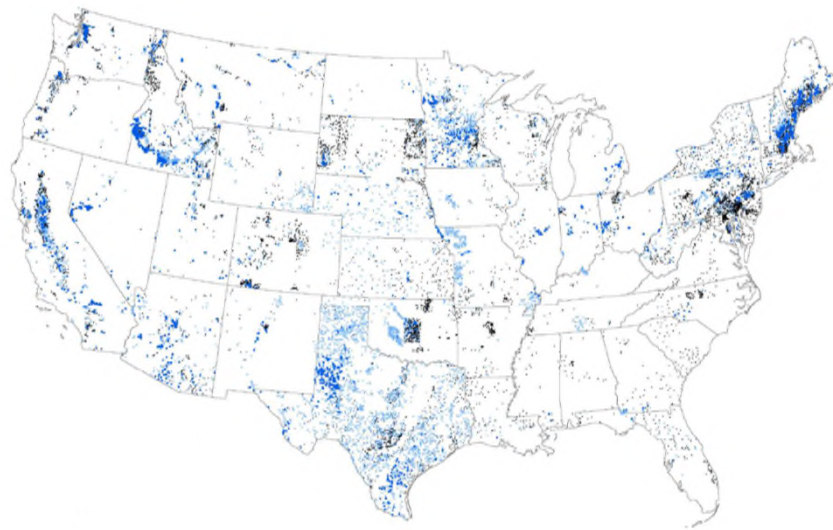- 0 - 0.05
- 0.05 - 0.15
- 0.15 - 0.3
- 0.3 - 0.5
- > 0.5

- Logistic Regression model

- Model response term is the probability of arsenic > 10μg/L

$$P(y|x) = \frac{e^{\beta_0+\beta_1 x_1 +\cdots+\beta_n x_n}}{1 + e^{\beta_0+\beta_1 x_1 +\cdots+\beta_n x_n}}$$

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Existing logistic regression model

Arsenic concentrations
from 20,450 domestic wells

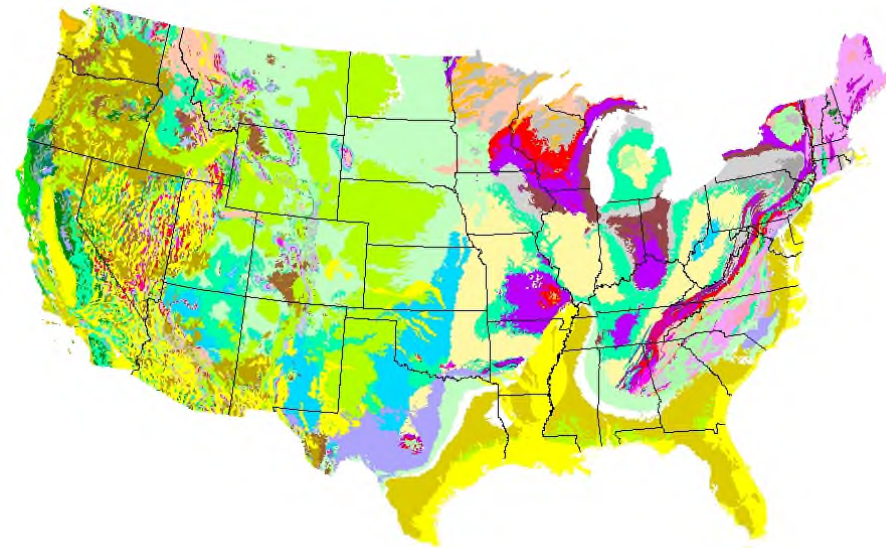Black = As < 1 μg/L
Light blue = 1 $\geq$ As < 10 μg/L
Dark blue = As > 10 μg/L

From Ayotte et al. 2017, ES&T
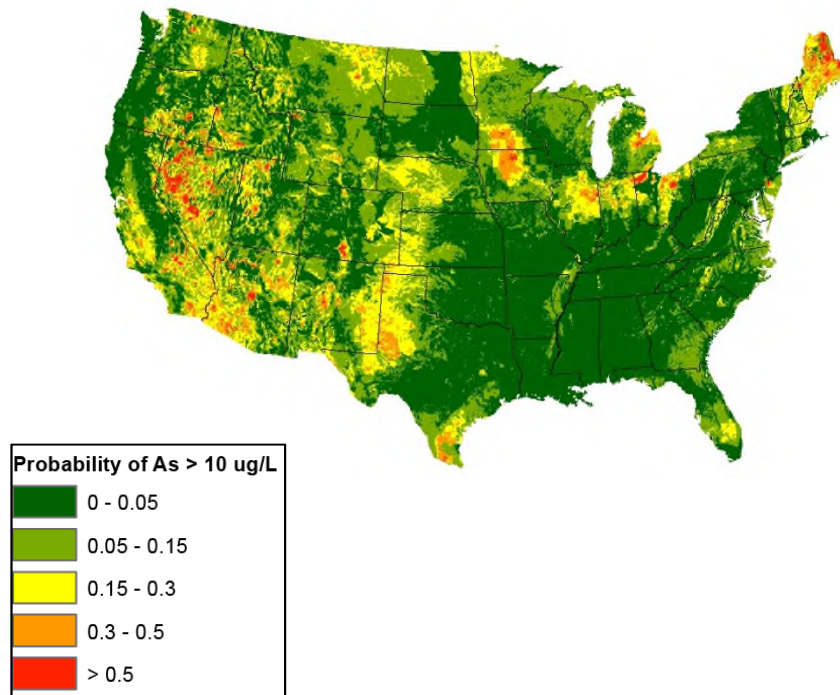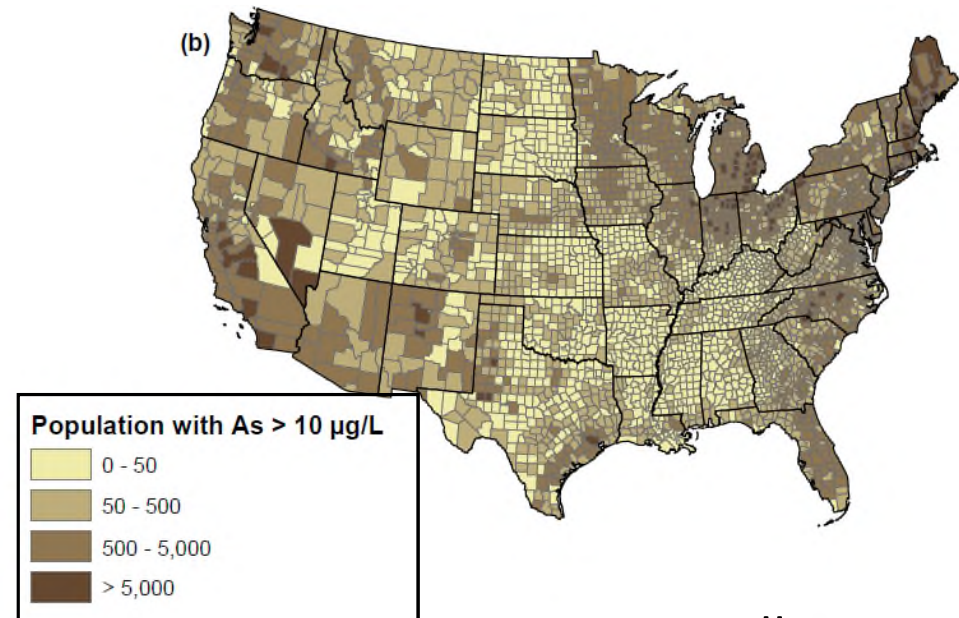
42 predictor variables

Generalized geology of the U.S.

After King and Beikman, 1974

Existing arsenic model and exposure estimate

Arsenic model output

Arsenic exposure estimate

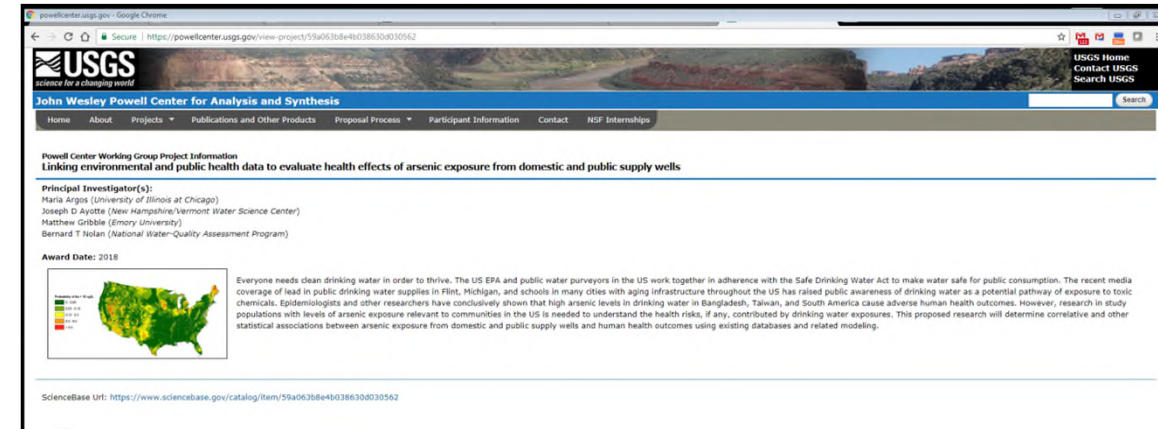Probability of As > 10 ug/L
- 0 - 0.05
- 0.05 - 0.15
- 0.15 - 0.3
- 0.3 - 0.5
- > 0.5

Population with As > 10 µg/L
- 0 - 50
- 50 - 500
- 500 - 5,000
- > 5,000

2.1 million people

From Ayotte et al. 2017, ES&T

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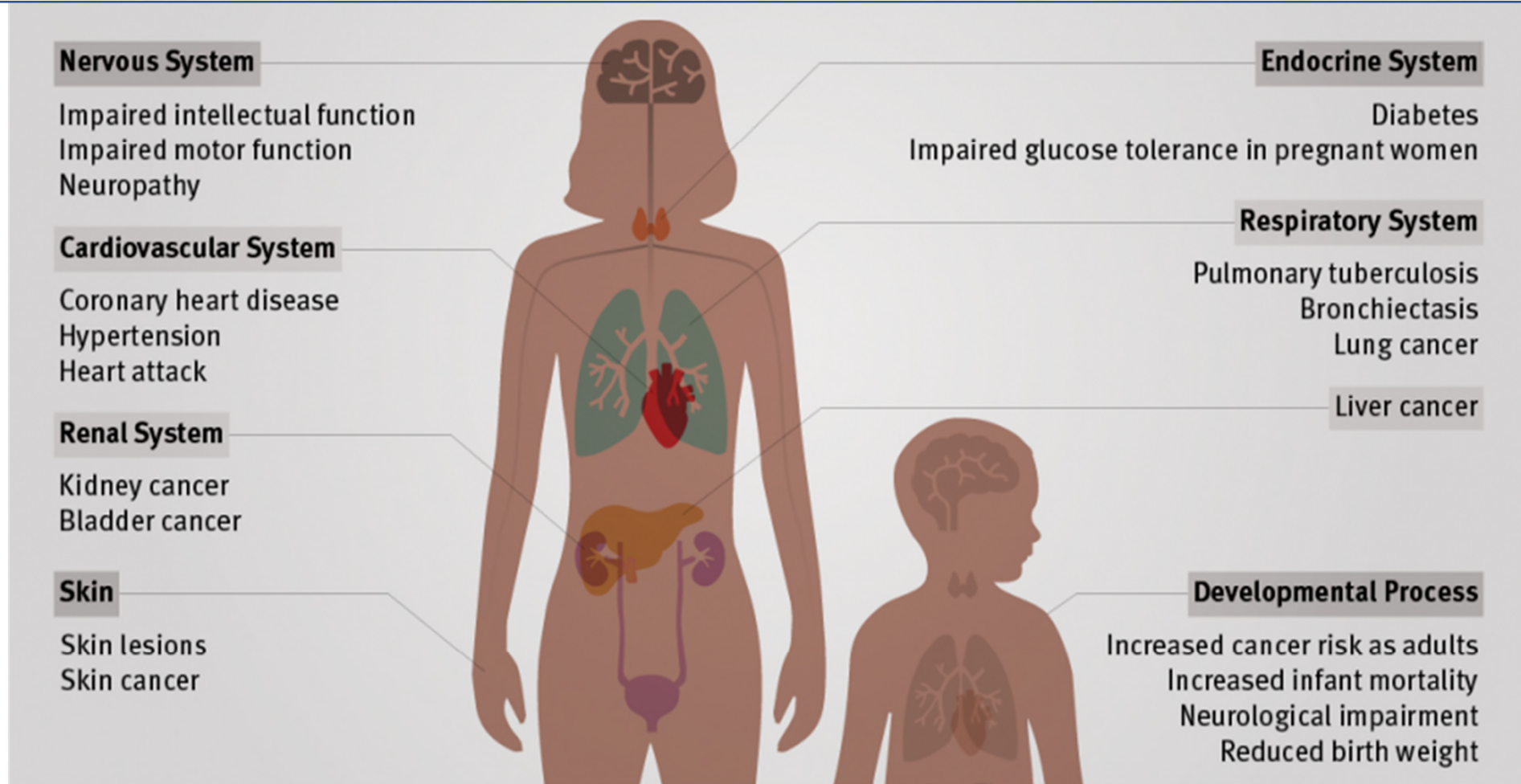*science for a changing world*

USGS Powell Center study

Linking environmental and public health data to evaluate health effects of arsenic exposure from domestic supply wells

- Make a new national arsenic model
  - Use machine learning methods
  - Update model variables

- Results will be used in epidemiology models to evaluate relationships between human health outcomes and arsenic in domestic wells.
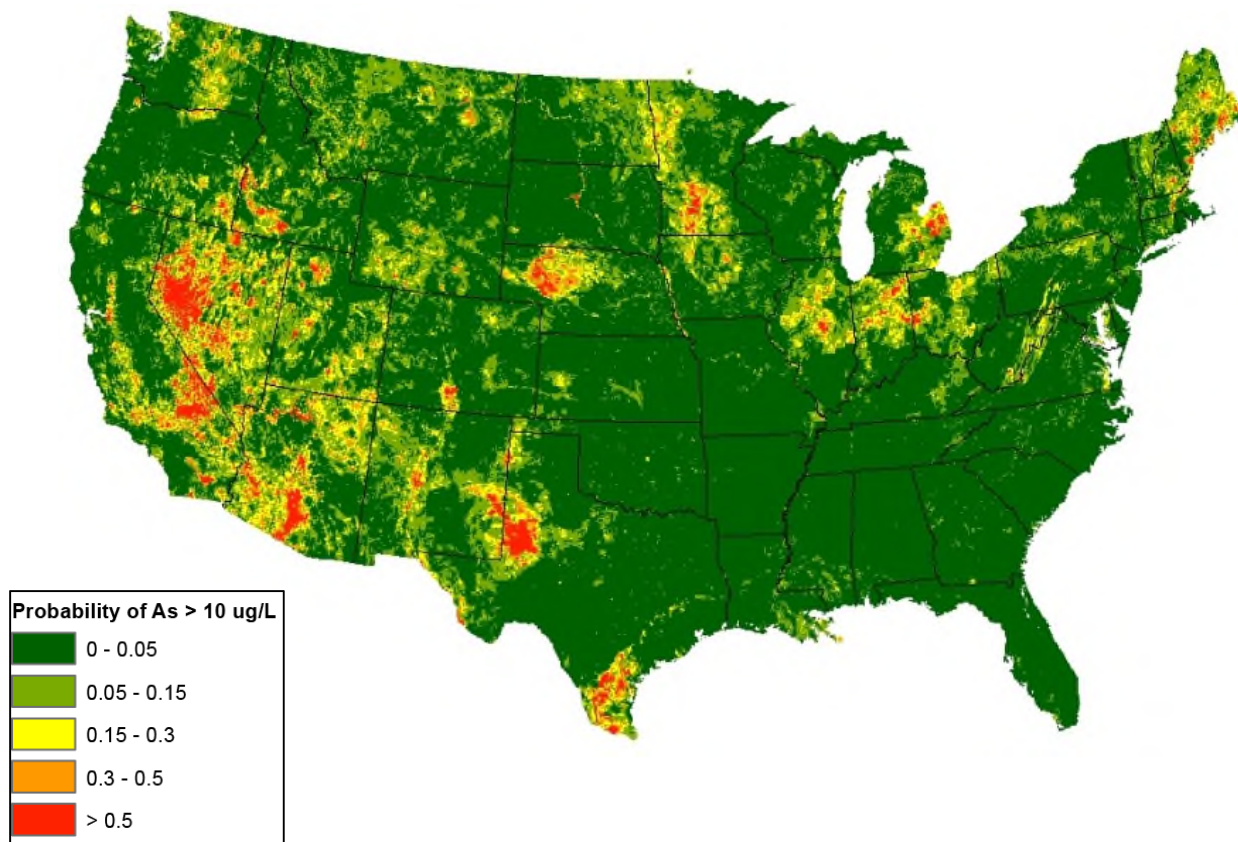
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Arsenic's effects on the human body

Nervous System

Impaired intellectual function
Impaired motor function
Neuropathy

Cardiovascular System

Coronary heart disease
Hypertension
Heart attack

Renal System

Kidney cancer
Bladder cancer

Skin

Skin lesions
Skin cancer

Endocrine System

Diabetes
Impaired glucose tolerance in pregnant women

Respiratory System

Pulmonary tuberculosis
Bronchiectasis
Lung cancer

Liver cancer

Developmental Process

Increased cancer risk as adults
Increased infant mortality
Neurological impairment
Reduced birth weight

https://www.hrw.org/report/2016/04/06/nepotism-and-neglect/failing-response-arsenic-drinking-water-bangladeshs-rural#page

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Boosted Regression Tree Model

Probability of As > 10 ug/L
- 0 - 0.05
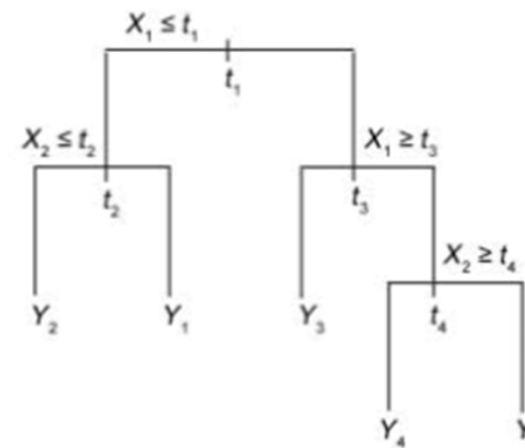- 0.05 - 0.15
- 0.15 - 0.3
- 0.3 - 0.5
- > 0.5

BRT Model
Number of trees = 4500
Interaction depth = 14
Learning rate = 0.01

From Elith et al., 2008

LR and BRT Model Comparison

LR Model

Probability of As > 10 ug/L
- 0 - 0.05
- 0.05 - 0.15
- 0.15 - 0.3
- 0.3 - 0.5
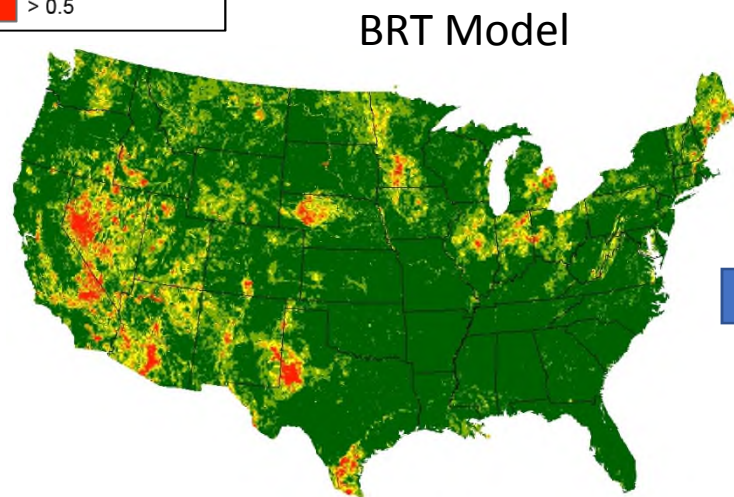- > 0.5

BRT Model

- Sharper delineation between high and low arsenic probabilities with BRT model

BRT minus LR probability

Change in Probability
- -1 - -0.4
- -0.4 - -0.2
- -0.2 - 0
- 0 − 0.4
- 0.4 - 1

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Model Comparison Predictive Performance

	Training Data			Hold-out Data		
	Accuracy	Sensitivity	Specificity	Accuracy	Sensitivity	Specificity
LR	89.9%	12.7%	99.3%	90.1%	13.9%	99.0%
BRT	95.6%	64.5%	99.3%	92.1%	43.7%	97.8%

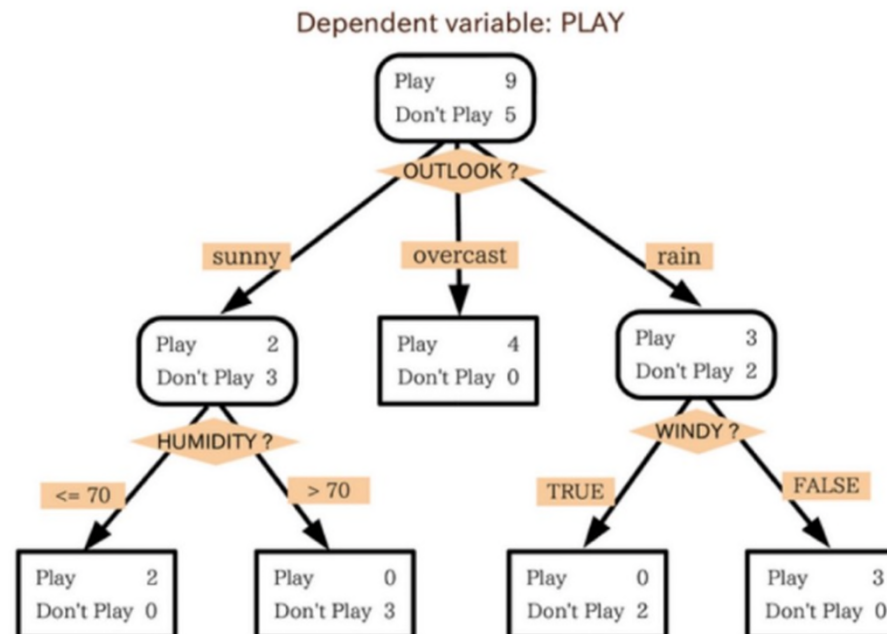Sensitivity = events (As>10μg/)   Specificity = non-events (As<10μg/L)

Random Forest Classification Model

- Ensemble tree based machine learning method

- Model response term is a classification (category)
  - Arsenic ≤ 10 μg/L
  - Arsenic > 10 μg/L
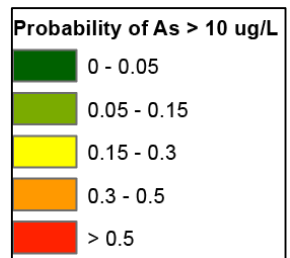
RFC Model
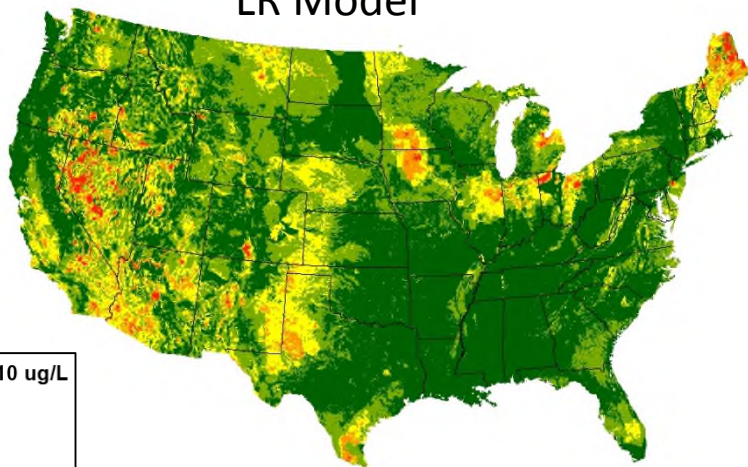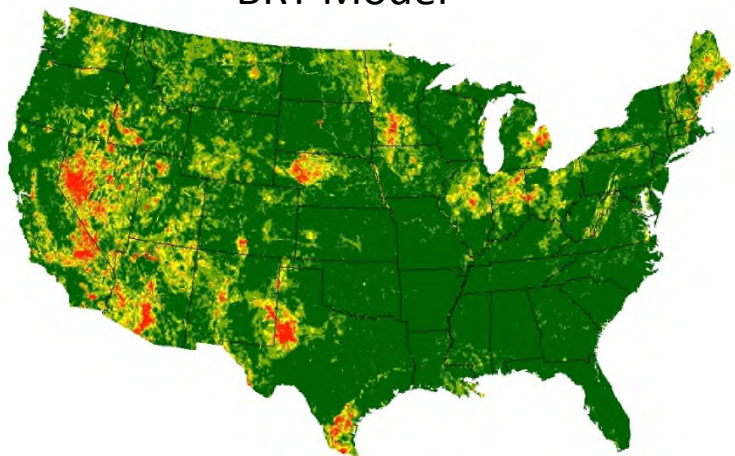Number of trees = 500
mtry = 38

Dependent variable: PLAY

From medium.com

LR, BRT, & RFC Model Comparison

LR Model

BRT Model

RFC Model

Probability of As > 10 ug/L
- 0 - 0.05
- 0.05 - 0.15
- 0.15 - 0.3
- 0.3 - 0.5
- > 0.5

Legend
- 1 Less than 10 ug/L
- 2 Greater than 10 ug/L

Model Comparison Predictive Performance

	Training Data			Hold-out Data		
	Accuracy	Sensitivity	Specificity	Accuracy	Sensitivity	Specificity
LR	89.9%	12.7%	99.3%	90.1%	13.9%	99.0%
BRT	95.6%	64.5%	99.3%	92.1%	43.7%	97.8%
RFC 2C	99.9%	100%	99.3%	91.0%	38.4%	97.1%

Sensitivity = events (As>10μg/L)
Classification As>10μg/L

Specificity = non-events (As<10μg/L)
Classification As<10μg/L

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Next steps

- Developing a RFC model with 4 concentration categories
  - ≤ 5 µg/L
  - 5 – 10 µg/L
  - 10 – 50 µg/L
  - > 50 µg/L

- Arsenic model results will be used in epidemiology models
  - Low birth weight
  - Cancers
  - Diabetes
  - Cardiovascular disease

Cancer Mortality Rates by State Economic Area (Age-adjusted 1970 US Population)
Bladder: White Males, 1970-94

US = 6.56/100,000

7.92-10.84 (highest 10%)
7.25- 7.91
6.81- 7.24
6.45- 6.80
6.14- 6.44
5.82- 6.13
5.41- 5.81
5.00- 5.40
4.68- 4.99
3.16- 4.67 (lowest 10%)

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Questions ?

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